

**DETERMINING STRUCTURES BY PERFORMING COMPARISONS
BETWEEN MOLECULAR REPLACEMENT RESULTS FOR
MULTIPLE DIFFERENT BIOMOLECULES**

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ABSTRACT

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A method is provided for identifying a search model to use in
molecular replacement for determining a structure of a target biomolecule,
such as a protein, from X-ray diffraction data, the method comprising:
employing computer executable logic to perform multiple molecular
15 replacement searches on X-ray diffraction data of the target biomolecule
where a group of different biomolecule structures are used as search models
for the multiple molecular replacement searches; and employing computer
executable logic to compare solutions from the multiple molecular
replacement searches, the comparison producing data from which biomolecule
20 structures can be identified as having superior structural identity with the
target biomolecule as compared to the other biomolecule structures in the
group.